substance: boron compounds with group III elements
property: properties of Al-B-C compounds

For conditions, structure and some properties of phases in the Al-B system see [79S]. For preparation, structures and some properties of Al-C-B compounds see [98M1].

Review of data on the equilibrium diagram of the Al-B system [89N].

Preparation and properties of high-dispersive powders of aluminium dodecaboride and carboborides [91K].

Preparation and characterization of compounds in the Al-B-C system [97M3].

For $Al_8B_4C_7$ see also Al_3BC_3.

For $Al_8B_{2-4}C_6$ see also Al_3BC_3.

Al_3BC

Preparation and structure [97M1, 97M2, 98M1].

Homogeneity range $Al_{2.6}B_{1.8}C$ – $Al_3B_{1.2}C$ [95P].

Superstructure:

Structure: trigonal

Space group: P3c1 98M1

Subcell:

Structure: hexagonal

Space group: $P6_3/mmc$ 98M1

Structure in Fig. 1 [98M1].

lattice parameters
(in Å)

superstructure

a	6.04	*T* = 300 K	X-ray diffraction	93G
c	11.54			
a	6.0345(12)	*T* = 300 K	X-ray diffraction	97M1,
c	11.520(2)			98M1

substructure

a	3.491(2)	*T* = 300 K	X-ray diffraction	92V
c	11.541(4)			
a	3.4849(9)	*T* = 300 K	X-ray diffraction	97M3
c	11.520(2)			

For the distances between the different atoms and further details of the structure see [98M1].

energy gap

E_g	~3 eV	calculated	98M1

Calculated electron density of states distribution in Fig. 2 [98M1].

COOP curves in Fig. 3 [98M1].

IR active phonon wavenumbers
(ν/c in cm^{-1})

ν/c	738	T = 300 K		98M1
	672			
	641			
	622			
	567			
	387			
	372			
	265			
	236			
	153			
	91			
	67			

Raman active phonon wavenumbers
(ν/c in cm^{-1})

ν/c	520	T = 300 K		98M1
	496			
	474			
	350			
	335			
	180			
	147			
	85			

IR and Raman spectrum in Fig. 4 [98M1].

density

d	2.658 g cm^{-3}	T =300 K	X-ray	98M1

Al_3BC_3

Al_3BC_3 – with the linear anion $[CBC]^{5-}$ [95H].

Synthesis, crystal structure and vibration spectra [96H2].

The structure can be described as a packing of Al_3C layers linked by linear C-B-C chains [96H1].

Superstructure: trigonal, space group: $P\bar{3}c1$

Subcell: hexagonal, space group: $P6_3/mmc$

Structure in Fig. 5 [98M1].

lattice parameters
(in Å)

superstructure

a	5.906	T = 300 K	X-ray diffraction ("$Al_8B_4C_7$")	80I
c	15.901			
a	5.903	T = 300 K	X-ray diffraction ("$Al_8B_{2-4}C_6$")	95O
c	15.92			
a	5.900(2)	T = 300 K	X-ray diffraction	96H1,
c	15.890(2)			98M1

substructure

a	3.4075(2)			98M1
c	15.900(2)			

For details of the structure, positions and distances between the atoms, see [98M1].

300 K equation of state and high-pressure phase stability of Al_3BC_3 [99S2].

energy gap

E_g	~5 eV		calculated	98M1

Calculated electron density of states distribution in Fig. 6 [98M1].

X-ray photoelectron spectrum (XPS) in Fig. 7 [98M1].

XANES spectrum in Fig. 8 [98M1].

IR active phonon wavenumbers
(ν/c in cm^{-1})

ν/c	1580	T = 300 K	asymm. valency vibr. of (CBC)	98M1
	1079			
	803			
	759			
	735			
	692			
	687			
	648			
	564			
	508			
	449		twofold degen. deform. vibr. of (CBC)	
	401			
	353			
	300			

Raman active phonon wavenumbers
(ν/c in cm^{-1})

ν	1490	T = 300 K	weak, estimated from diagram	96H1
	1470		weak, estimated from diagram	98M1
	1120		weak, estimated from diagram	
	1041		symm. valency vibr. of (CBC)	
	1010		weak, estimated from diagram	
	720		weak, estimated from diagram	
	680		weak, estimated from diagram	
	581			
	559			
	521			
	421			
	358			
	276			
	248			
	117			

IR transmission and FT-Raman spectrum in Fig. 9 [96H1].

density

d	2.658 g cm^{-3}	*T* = 300 K	X-ray	98M1

$Al_4B_xC_{3-x}$ (x = ..6)

Space group: $R\bar{3}m$

Structure in Fig. 10 [97M1, 98M1].

Preparation and structure [97M1].

lattice parameters

a	3.34954 Å	*T* = 300 K	X-ray diffraction	97M1,
c	24.951(3) Å			98M1

Optical transmission spectrum in the absorption edge range in Fig. 11 [97M1].

IR active phonon wavenumbers
(*ν*/*c* in cm^{-1})

	$Al_4B_{0.5}C_{2.5}$	$Al_4B_{0.5}{}^{13}C_{2.5}$		
ν/*c*	826	798	*T* = 300 K	97M1
	780			98M1
	740	715		
	609	605		
	506	509		
	454	461		
	426	421		
	351	346		
	179	182		
	120	120		

Raman active phonon wavenumber
(*ν*/*c* in cm^{-1})

	$Al_4B_{0.5}C_{2.5}$	$Al_4B_{0.5}{}^{13}C_{2.5}$		
ν/*c*	856	828	*T* = 300 K	98M2
		785		
	709	688		98M1
		644		
	614	604		
	490	487		
		436		
	428	419		
	341	340		
	297	298		
	252	250		

IR transmission spectrum in the range and FT-Raman spectrum of phonon frequencies in Fig. 12 [97M1].

References:

79S Samsonov, G.V., Neronov, V.A., Lamikhov, L.K.: J. Less-Common Met. 67 (1979) 291.

80I Inoue, Z., Tanaka, H., Inomata, Y.: J. Mater. Sci. 15 (1980) 3036.

89N Neronov, V.A.: Sov. Powder Metall. Met. Ceram. 28 (1989) 789.

91K Kharlamov, A.I., Duda, T.I., Fomenko, V.V.: in: Boron-Rich Solids, Proc. 10th Int. Symp. Boron, Borides and Rel. Compounds, Albuquerque, NM 1990 (AIP Conf. Proc. 231), D. Emin, T.L. Aselage, A.C. Switendick, B. Morosin, C.L. Beckel ed., American Institute of Physics: New York, 1991, p. 512.

92V Viala, J.C., Gonzales, G., Bouix, J.: J. Mater. Sci. Lett. 11 (1992) 711.

93G Gonzalez, G., Esnouf, C., Viala, J.C.: Mater Sci. Forum 126-128 (1993) 125.

95H Hillebrecht, H., Meyer, F.D.: Z. Kristallogr. Suppl. 9 (1995) 176.

95O Oscroft, R.J., Roebuck, P.H.A., Thompson, D.P.: Br. Ceram. Trans. 94 (1995) 25.

95P Paderno, Y., Shitsevalova, N., Bat'ko, I., Flachbart, K., Misiorek, H., Mucha, J., Jezowski, A.: J. Alloys Compounds 219 (1995) 215.

96H1 Hillebrecht, H., Meyer, F.D.: Angew. Chem. Int. Ed. Engl. 35 (1996) 2499.

96H2 Hillebrecht, H., Meyer, F.D.: Angew. Chem. 108 (1996) 2655.

97M1 Meyer, F.D., Hillebrecht, H.: Z. Kristallogr. Suppl. 12 (1997) 127.

97M2 Meyer, F.D., Hillebrecht, H.: J. Alloys Compounds 252 (1997) 98.

97M3 Meyer, F.D., Hillebrecht, H.: in: Jahresbericht 1996 des Freiburger Materialforschungszentrums FMF, Albert-Ludwigs-Universität, Freiburg, University of Freiburg ed., Freiburg, 1997, p. 55.

98M1 Meyer, F.D.: in: Thesis, Albert-Ludwigs-Universität Freiburg ed., Freiburg, Germany, 1998 .

98M2 Medwick, P.A., White Jr., B.E., Pohl, R.O.: J. Alloys Compounds 270 (1998) 1.

99S1 Saillard, J.-Y., Halet, J.-F., Gautier, R., Meyer, F., Hillebrecht, H.: (in preparation).

99S2 Solozhenko, V.L., Meyer, F.D., Hillebrecht, H.: J. Solid State Chem. (2000) (Proc. 13th Int. Symp. Boron, Borides and Rel. Compounds, Dinard, France, Sept. 1999).

99Z Zaoui, A., Certier, M., Ferhat, M., Paés, O., Aourag, H.: Phys. Status Solidi (b) 212 (1999) 307.

Fig. 1.

Al_3BC. Crystal structure. Model of the subcell in $P6_3/mmc$. The disorder of the Al(2) atoms in *c* direction is not considered. **(a)** sphere-bar model; **(b)** polyeder representation of the Al(1)-centered AlC_4 tetrahedra [98M1].

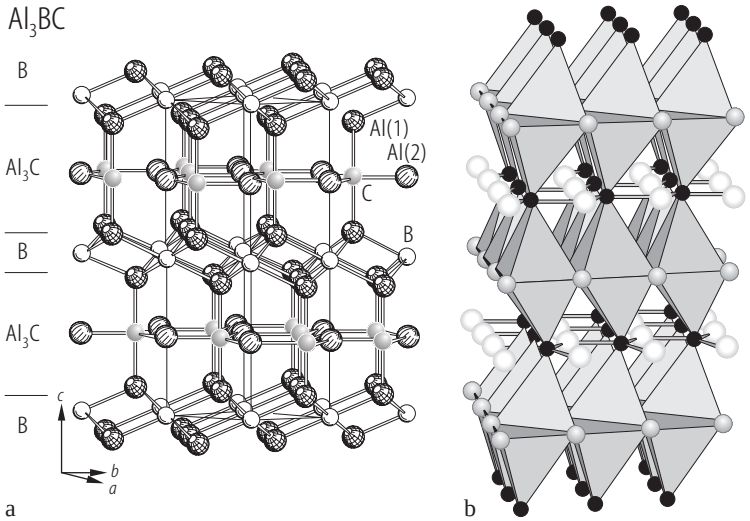

Fig. 2.

Al_3BC. Electron total and partial density of states obtained with the Extended Hückel Method [98M1, 99S1]. Number of states is also shown in lower part

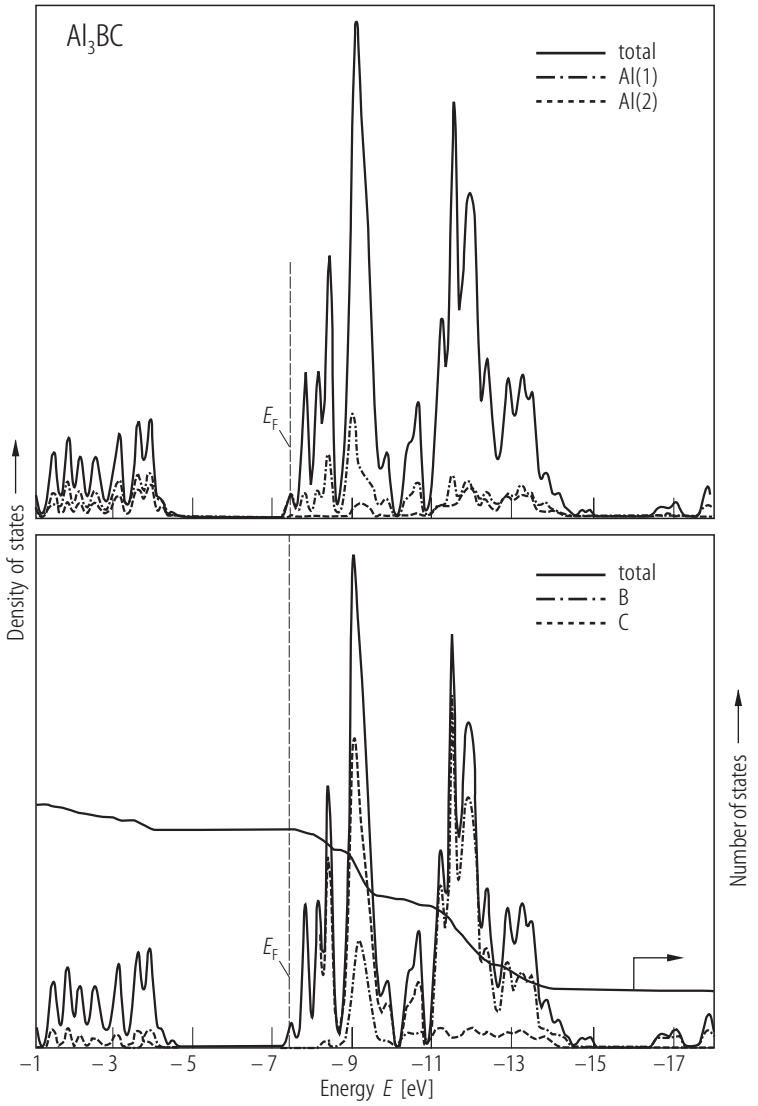

Fig. 3.

Al_3BC. COOP (Crystal orbital overlap population) curves attributed to the bonds Al-B, Al-Al and Al-C [98M1, 99S1].

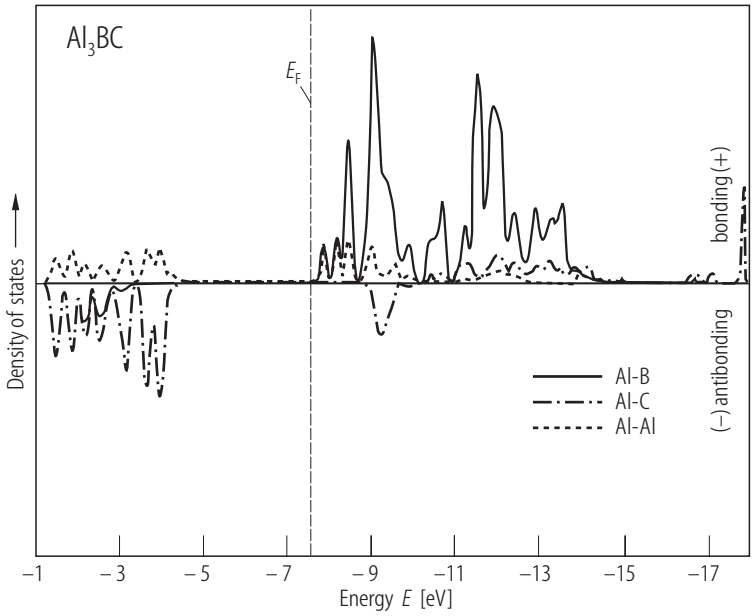

Fig. 4.

Al_3BC. Phonon spectra (IR and Raman) obtained by FT spectroscopy [98M1].

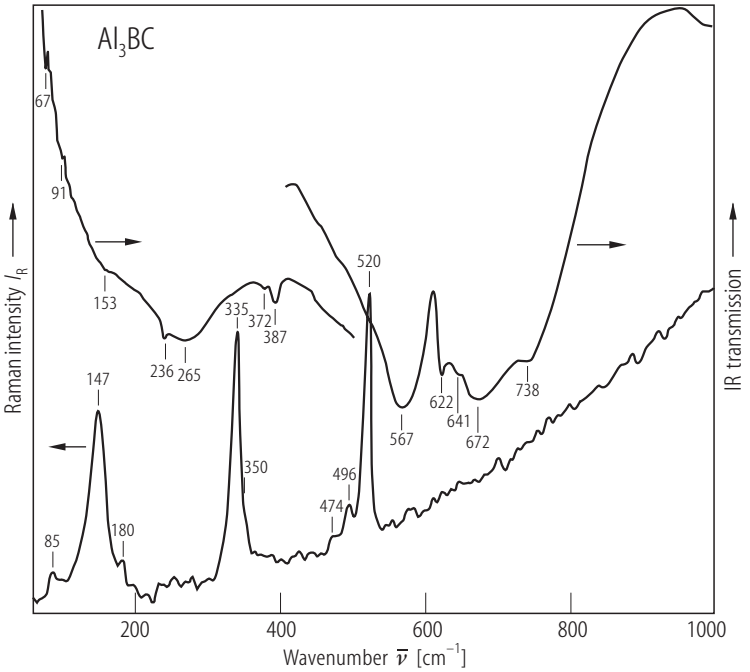

Fig. 5.

Al_3BC_3. Crystal structure, model of the subcell in $P6_3/mmc$. The disorder of the Al(1) atoms in *c* direction is not considered. **(a)** sphere-bar model; **(b)** polyhedral representation of the Al-centered AlC_4 tetrahedra. [98M1].

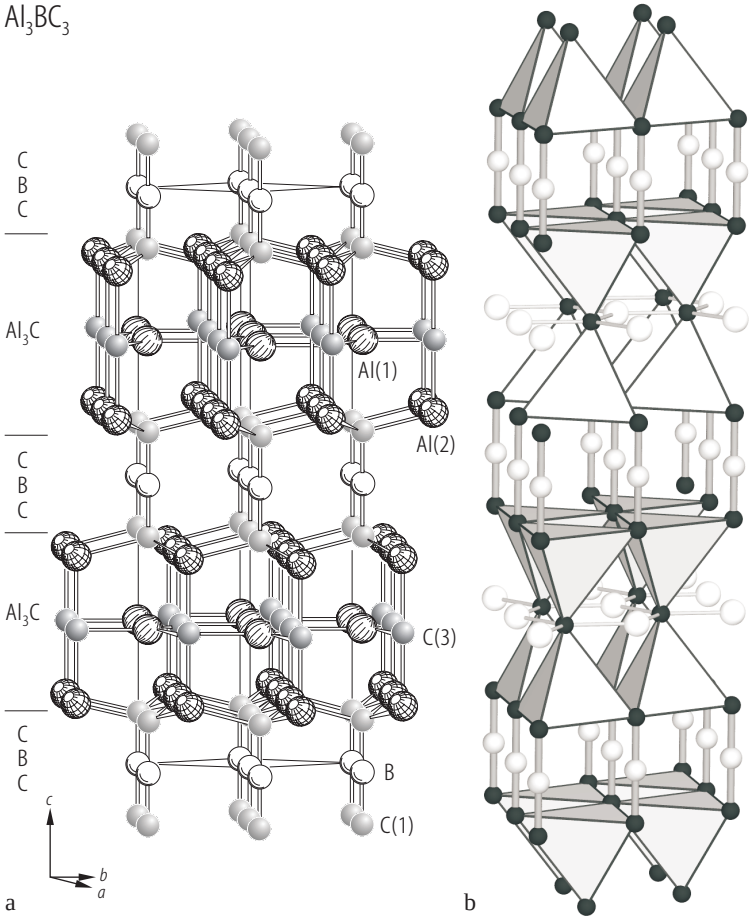

Fig. 6.

Al_3BC_3. Total and partial electron densities of states obtained with the Extended Hückel Method) (calculated by Meyer, Hillebrecht,Saillard, Halet and Gautier) [98M1, 99S1].

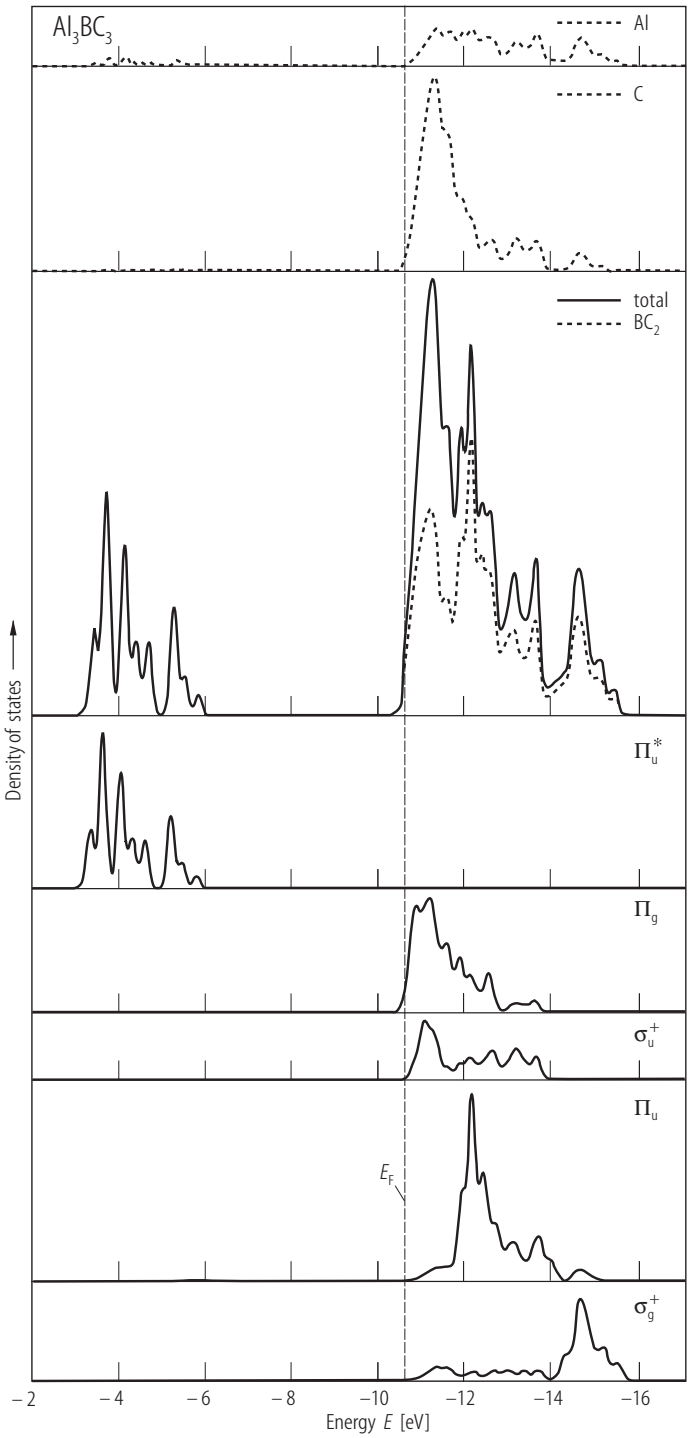

Fig. 7.

Al_3BC_3. X-ray photoelectron spectrum (XPS) [98M1].

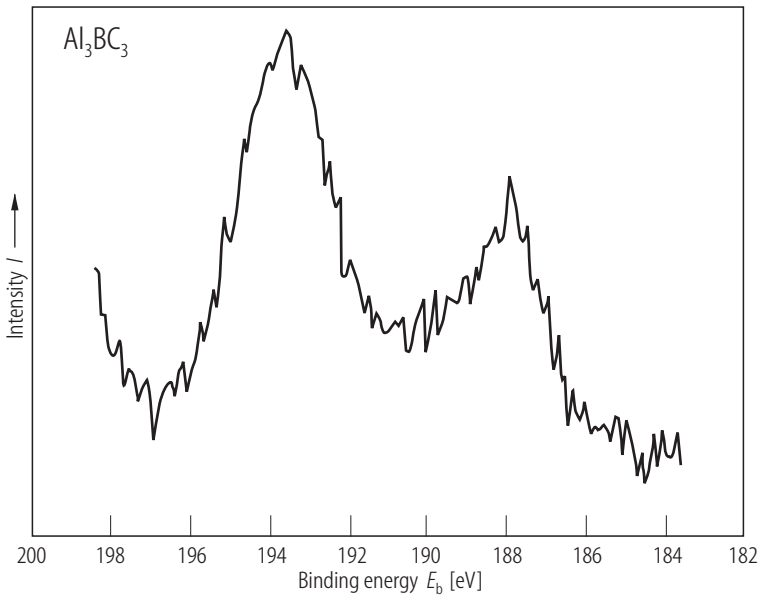

Fig. 8.

Al_3BC_3. XANES spectrum compared with those of some other boron compounds (boron carbide, B_2O_3, hexagonal BN) [98M1].

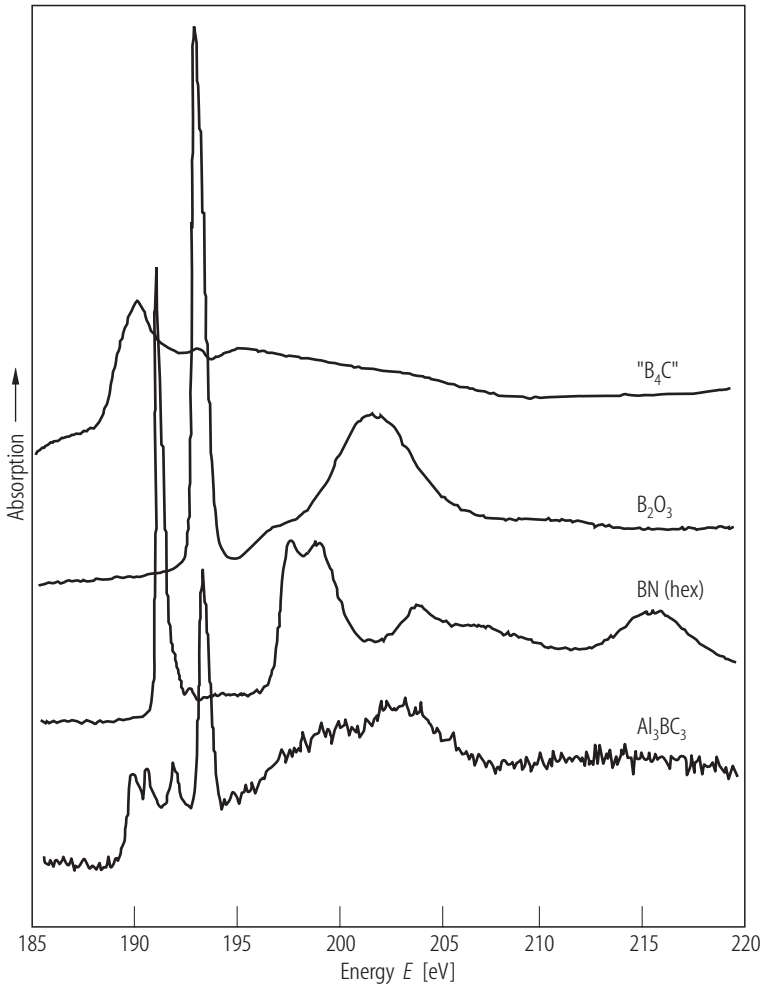

Fig. 9.

Al_3BC_3. IR transmission and FT-Raman spectrum [96H1, 98M1].

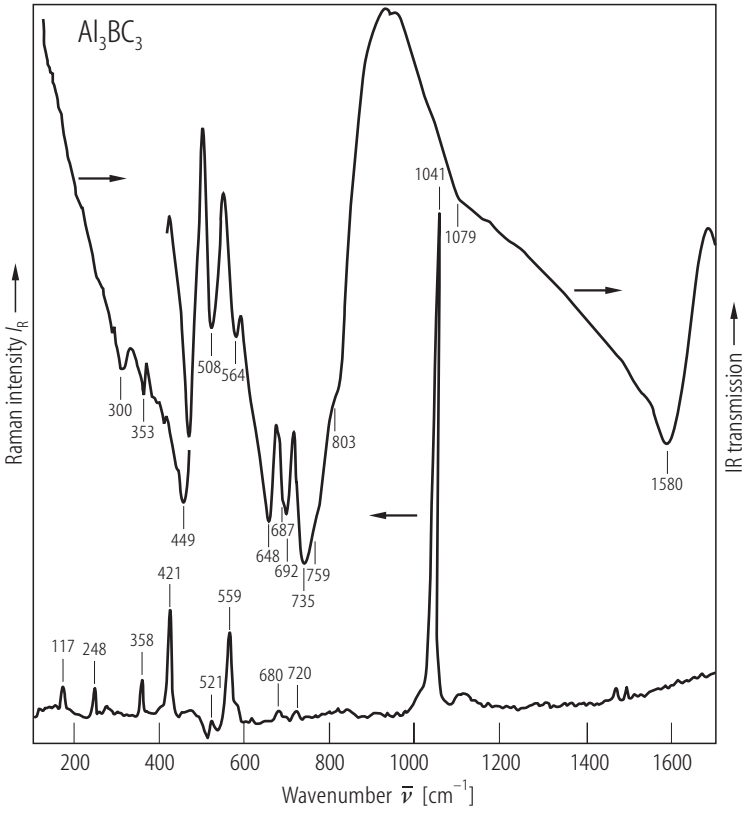

Fig. 10.

$Al_4B_xC_{3-x}$. Structure with marked elementary cell [98M1]. Al(2) atoms are disordered.

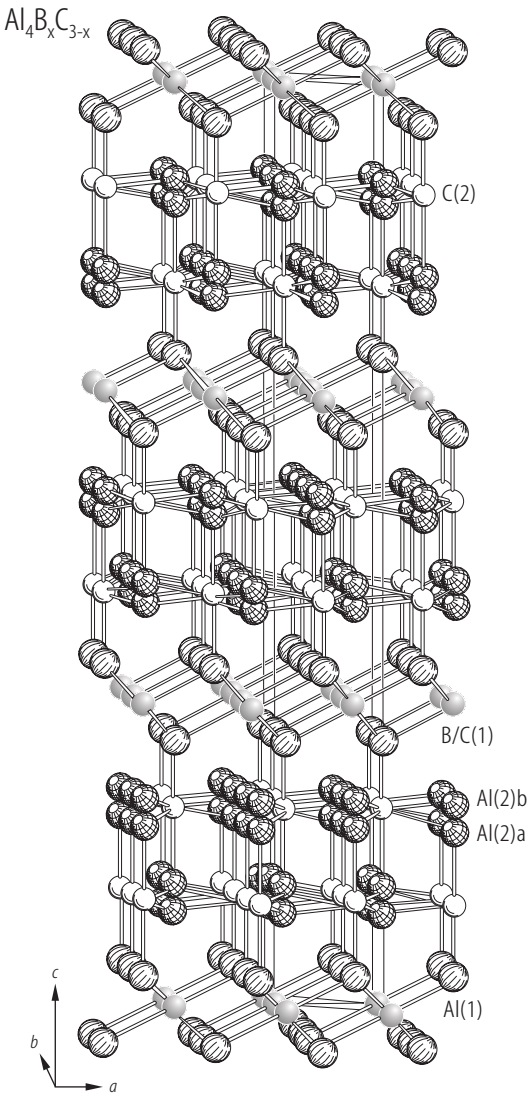

Fig. 11.

$Al_4B_{0.5}C_{2.5}$. Optical transmission spectrum in the absorption edge range [97M1].

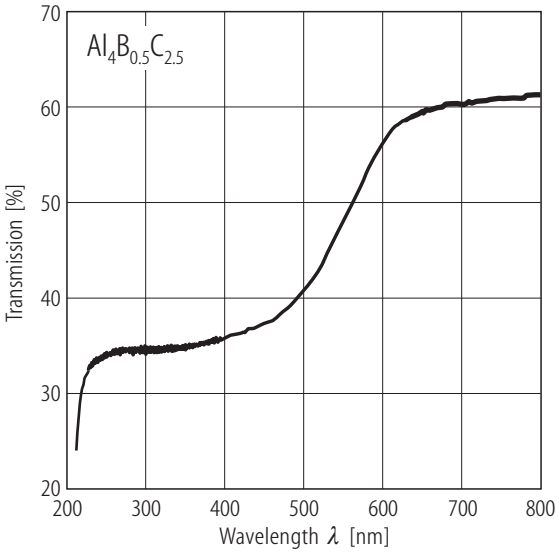

Fig. 12.

$Al_4B_{0.5}C_{2.5}$. Optical trans-mission spectrum and FT Raman spectrum in the range of phonon frequencies [97M1]. Remark: the step in the IR spectrum at about 180 cm^{-1} is probably not real but due to the change of the spectral range of the FTIR spectrometer.